

**Isolation of a C-5-Deprotontonated Imidazolium, a Crystalline  
“Abnormal” N-Heterocyclic Carbene**

Eugenia Aldeco-Perez,<sup>1</sup> Amos J. Rosenthal,<sup>1</sup> Bruno Donnadieu,<sup>1</sup> Pattiyl Parameswaran,<sup>2</sup> Gernot Frenking,<sup>2</sup> Guy Bertrand<sup>1\*</sup>

<sup>1</sup>UCR-CNRS Joint Research Chemistry Laboratory (UMI 2957)

Department of Chemistry, University of California  
Riverside, CA 92521-0403, USA

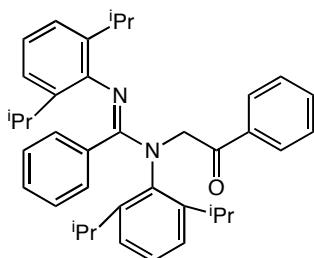
<sup>2</sup>Fachbereich Chemie, Philipps-Universitat Marburg, Hans-Meerwein-Strasse,  
35032 Marburg, Germany

**SUPPORTING INFORMATION**

## Synthesis and Spectroscopic Data

All experiments were carried out under dry argon using standard Schlenk or dry box techniques. Solvents were dried by standard methods and distilled under argon. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded on Varian Inova 400, 500 and Brucker 300 spectrometers at 25 °C and referenced to the residual <sup>1</sup>H, and <sup>13</sup>C signals of the solvents. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, sept. = septet, m = multiplet, br = broad signal. Coupling constants *J* are given in Hz. Mass spectra were performed at the UC Riverside Mass Spectrometry Laboratory. Melting points were measured with a Büchi melting point apparatus system.

### N,N' bis (2, 6-diisopropylphenyl)-N-(2-oxo-2-phenylethyl)benzimidamide



An isopropanol solution (30 mL) of N, N'-bis(2,6-diisopropylphenyl)benzimidamide (*SI*) (10 g, 21 mmol), 2-bromoacetophenone (4.5 g, 23 mmol) and potassium bicarbonate (5 g, 50 mmol) was heated under reflux for 24 hours. Filtration of the potassium bicarbonate and evaporation of the solvent gave an oil. After adding hexane (20 mL), the solution was heated under reflux for 5 minutes, and a white precipitate was obtained by cooling down to 0 °C. Recrystallization from ethanol afforded the title compound as colorless crystals (7.6 g, 60% yield).

M.p. 142-143°C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 25 °C, 300 MHz): 8.05 (d, *J* = 8 Hz, 2 H, CH<sub>ar</sub>), 7.55-7.14 (m, 4 H, CH<sub>ar</sub>), 7.07-6.79 (m, 10 H, CH<sub>ar</sub>), 5.04 (s, 2 H, CH<sub>2</sub>), 4.59 (sept, *J* = 6.7 Hz, 2 H, CHCH<sub>3</sub>), 3.16 (sept, *J* = 6.7 Hz, 2 H, CHCH<sub>3</sub>), 1.26 (d, *J* = 7 Hz, 12 H, CH<sub>3</sub>), 1.06 (d, *J* = 7 Hz, 6 H, CH<sub>3</sub>), 0.97 (d, *J* = 7 Hz, 6 H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 25 °C, 75 MHz): 193.2 (CO), 156.4 (C=N), 147.8 (C<sub>ar</sub>), 144.8 (C<sub>ar</sub>), 140.6 (C<sub>ar</sub>), 138.7 (C<sub>ar</sub>), 136.7 (C<sub>ar</sub>), 132.9 (CH<sub>ar</sub>), 132.4 (C<sub>ar</sub>), 128.9 (CH<sub>ar</sub>), 128.7 (CH<sub>ar</sub>), 128.5 (CH<sub>ar</sub>), 127.9 (CH<sub>ar</sub>), 127.1 (CH<sub>ar</sub>), 124.3 (CH<sub>ar</sub>), 122.5 (CH<sub>ar</sub>), 122.1 (CH<sub>ar</sub>), 58.2 (CH<sub>2</sub>), 28.3 (CHCH<sub>3</sub>), 28.0 (CHCH<sub>3</sub>), 26.5 (CH<sub>3</sub>), 25.0 (CH<sub>3</sub>), 23.0 (CH<sub>3</sub>), 22.3 (CH<sub>3</sub>); HRMS: m/z calculated for C<sub>39</sub>H<sub>47</sub>N<sub>2</sub>O 559.3683, found 559.3694.

### N,N'-Bis(1,3-bis(2,6-diisopropylphenyl)-2,4-diphenylimidazolium 6(BF<sub>4</sub>)

HBF<sub>4</sub>·OEt<sub>2</sub> (1.4 mL, 10.2 mmol) was added dropwise at 0 °C to a suspension of N, N'-bis(2,6-diisopropylphenyl)-N-(2-oxo-2-phenylethyl)benzimidamide (1.75 g, 3.1 mmol) in acetic anhydride (2 ml). The mixture was warmed to room temperature and stirred overnight. Water (20 mL) and then CH<sub>2</sub>Cl<sub>2</sub> (20mL) were added at 0 °C. The organic layer was separated, washed with water (3 x 20 mL), and dried with anhydrous MgSO<sub>4</sub>. After evaporation of the solvent under vacuum, the residue was

washed with Et<sub>2</sub>O, giving **6**(BF<sub>4</sub><sup>-</sup>) as a white solid. Recrystallization in CHCl<sub>3</sub>/hexane afforded colorless crystals (1.75g, 90% yield).

M.p. 242-243°C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 25 °C, 300 MHz): 8.31 (s, 1 H, CH<sub>imidazolium</sub>), 7.66-7.41 (m, 2 H, CH<sub>ar</sub>), 7.40-7.23 (m, 12 H, CH<sub>ar</sub>), 6.95 (d, *J* = 9 Hz, 2 H, CH<sub>ar</sub>), 2.56-2.46 (m, 4 H, CHCH<sub>3</sub>), 1.35 (d, *J* = 6.6 Hz, 6 H, CH<sub>3</sub>), 1.01 (d, *J* = 6.6 Hz, 6 H, CH<sub>3</sub>), 0.86 (br, 12 H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 25 °C, 100 MHz): 145.5 (C), 145.2 (C), 144.8 (C), 137.4 (C), 133.1 (CH<sub>ar</sub>), 133.0 (CH<sub>ar</sub>), 132.6 (CH<sub>ar</sub>), 131.0 (CH<sub>ar</sub>), 130.3 (C), 129.9 (CH<sub>ar</sub>), 129.7 (CH<sub>ar</sub>), 129.4 (CH<sub>ar</sub>), 128.8 (CH<sub>ar</sub>), 128.8 (C), 126.3 (CH<sub>ar</sub>), 125.6 (CH<sub>ar</sub>), 124.5 (C), 123.2 (CH<sub>imidazolium</sub>), 121.0 (C), 29.4 (CHCH<sub>3</sub>), 29.1 (CHCH<sub>3</sub>), 25.3 (CH<sub>3</sub>), 23.7 (CH<sub>3</sub>), 23.3 (CH<sub>3</sub>), 22.5 (CH<sub>3</sub>); HRMS: m/z calculated for C<sub>39</sub>H<sub>45</sub>N<sub>2</sub> 541.3577 , found M 541.3578 .

### **1,3-bis(2,6-diisopropylphenyl)-2,4-diphenyl-imidazolium 6(HBr<sub>2</sub>)**

Using the same procedure as for the tetrafluoroborate imidazolium salt **6**(BF<sub>4</sub><sup>-</sup>), but HBr (48% in water). Quantities were the following: N,N'-bis(2,6-diisopropylphenyl)-N-(2-oxo-2-phenylethyl)benzimidamide (2.1 g, 3.7 mmol), HBr 48% (2 mL, 17 mmol). **6**(HBr<sub>2</sub>) was isolated as a white solid (2.6 g, 100% yield).

m.p. 207-209°C; HRMS: m/z calculated for C<sub>39</sub>H<sub>45</sub>N<sub>2</sub> 541.3577, found 541.3583.

Recrystallization from dichloromethane/hexane at room temperature afforded a few single crystals of **6**(Br<sup>-</sup>).

### **1,3-bis(2,6-diisopropylphenyl)-2,4-diphenyl-imidazolium 6(HCl<sub>2</sub>)**

Using the same procedure as for the tetrafluoroborate imidazolium salt **6**(BF<sub>4</sub><sup>-</sup>), but HCl (12.1M in water). Quantities were the following: N,N'-bis(2,6-diisopropylphenyl)-N-(2-oxo-2-phenylethyl)benzimidamide (1 g, 1.9 mmol), HCl (1 mL, 12 mmol). **6**(HCl<sub>2</sub>) was obtained as a white solid (1.1 g, 95% yield).

m.p. 189-191°C.

### **aNHC lithium adduct 7**

THF (4 mL) was added at -78°C to a mixture of imidazolium salt **6**(HCl<sub>2</sub>) (341 mg, 0.56 mmol) and lithium diisopropylamide (119 mg, 1.11 mmol). After 30 min at -78°C, the mixture was warmed to room temperature and stirred during 2 hours. Solvent was evaporated under vacuum and the residue was extracted with hexane (3 x 20 mL). Removal of the solvent under vacuum afforded adduct **7** as a green oil (75 mg, 23% yield).

<sup>1</sup>H NMR (C<sub>6</sub>D<sub>6</sub>, 25°C, 400 MHz): 7.92 (d, *J* = 8.4 Hz, 2 H, CH<sub>ar</sub>), 7.17-6.87 (m, 12 H, CH<sub>ar</sub>), 6.61-6.60 (m, 2 H, CH<sub>ar</sub>), 3.18 (sept, *J* = 6.4 Hz, 2 H, CHCH<sub>3</sub>), 2.88 (sept, *J* = 6.4 Hz, 2 H, CHCH<sub>3</sub>), 1.35 (d, *J* = 6.4 Hz, 6 H, CH<sub>3</sub>), 0.97 (d, *J* = 6.4 Hz, 6 H, CH<sub>3</sub>), 0.80 (d, *J* = 6.4 Hz, 6 H, CH<sub>3</sub>), 0.74 (d, *J* = 6.4 Hz, 6 H, CH<sub>3</sub>); <sup>13</sup>C NMR (C<sub>6</sub>D<sub>6</sub>, 25°C, 100 MHz): <sup>13</sup>C NMR (THF, 25°C, 125 MHz): 190 (br, CLi), 144.6 (C), 144.3 (C), 144.1 (C), 140.9 (C), 138.2 (C), 134.1(C), 132.4 (C), 130.0 (CH<sub>ar</sub>), 129.0 (CH<sub>ar</sub>), 128.7 (CH<sub>ar</sub>), 128.5 (CH<sub>ar</sub>), 128.3 (CH<sub>ar</sub>), 127.4 (CH<sub>ar</sub>), 127.0 (CH<sub>ar</sub>), 125.3 (CH<sub>ar</sub>), 124.6 (CH<sub>ar</sub>), 123.3 (CH<sub>ar</sub>), 28.2 (CHCH<sub>3</sub>), 27.9 (CHCH<sub>3</sub>), 24.2 (CH<sub>3</sub>), 22.8 (CH<sub>3</sub>), 22.5 (CH<sub>3</sub>), 21.6 (CH<sub>3</sub>).

**1-(2,6-diisopropylphenyl)-5-isopropyl-9,9-dimethyl-2,9a-diphenyl-9,9a-dihydro-1*H*-imidazo[1,2-*a*]indole 8**

THF (6 mL) was added at -78°C to a mixture of imidazolium salt **6**(HBr<sub>2</sub><sup>-</sup>) (580 mg, 0.82 mmol) and lithium diisopropylamide (170 mg, 1.6 mmol). After 30 min at -78°C, the mixture was warmed to room temperature and stirred during 2 hours. The solvent was evaporated under vacuum, and the residue dissolved in 10 mL of Et<sub>2</sub>O. 12-Crown-4 (0.26mL) was added dropwise, and a white precipitate appeared immediately. After filtration, the ether solution was concentrated under vacuum affording a brown oil (200 mg, 45 % yield). Colorless single crystals of **8** were obtained from a concentrated Et<sub>2</sub>O/hexane solution at -20 °C.

<sup>1</sup>H NMR (C<sub>6</sub>D<sub>6</sub>, 25 °C, 400 MHz): 7.09-6.63 (m, 16 H, CH<sub>ar</sub>), 6.39 (s, 1 H, CH<sub>imidazolium</sub>), 4.32 (sept, *J* = 6.8 Hz, 1 H, CHCH<sub>3</sub>), 3.51 (sept, *J* = 6.8 Hz, 2 H, CHCH<sub>3</sub>), 1.94 (s, 3 H, CH<sub>3</sub>), 1.43 (d, *J* = 6.8 Hz, 3 H, CH<sub>3</sub>), 1.32 (d, *J* = 7.2 Hz, 3 H, CH<sub>3</sub>), 1.26 (d, *J* = 6.4 Hz, 3 H, CH<sub>3</sub>), 1.22 (d, *J* = 6.4 Hz, 3 H, CH<sub>3</sub>), 1.03-1.02 (m, 6 H, CH<sub>3</sub>), 0.15 (d, *J* = 6.4 Hz, 3 H, CH<sub>3</sub>); <sup>13</sup>C NMR (C<sub>6</sub>D<sub>6</sub>, 25°C, 100 MHz): 152.3 (C), 150.8 (C), 144.9 (C), 143.4 (C), 141.0 (C), 137.7 (C), 137.7 (C), 136.5 (C), 133.6 (C), 128.9 (CH<sub>ar</sub>), 128.5 (CH<sub>ar</sub>), 127.1 (CH<sub>ar</sub>), 126.9 (CH<sub>ar</sub>), 126.2 (CH<sub>ar</sub>), 126.0 (CH<sub>ar</sub>), 125.4 (CH<sub>ar</sub>), 124.3 (CH<sub>ar</sub>), 121.4 (CH<sub>ar</sub>), 121.1 (CH<sub>ar</sub>), 104.1 (NCN), 55.2 (C), 30.6 (CH<sub>3</sub>), 29.0 (CHCH<sub>3</sub>), 28.5 (CHCH<sub>3</sub>), 28.2 (CHCH<sub>3</sub>), 25.7 (CH<sub>3</sub>), 25.3 (CH<sub>3</sub>), 25.2 (CH<sub>3</sub>), 24.7 (CH<sub>3</sub>), 24.4 (CH<sub>3</sub>), 24.0 (CH<sub>3</sub>).

**Synthesis of the free *a*NHC 9**

Imidazolium salt **6**(HCl<sub>2</sub><sup>-</sup>) (800 mg, 1.3 mmol) and potassium hexamethyldisilazide (520 mg, 2.6 mmol) were dissolved in THF at -78°C and stirred during 30 minutes. The mixture was then warmed to room temperature and stirred during 2 hours. The solvent was removed under vacuum, and the residue extracted with hexane (2 x 20 mL). After filtration, the solvent was removed under vacuum, affording **9** as a green powder (480 mg, 68 % yield). Single yellow crystals of **9** were grown from hexane at -78°C. *a*NHC **9** is stable at room temperature for a few days under a strict argon atmosphere.

M.p. 65 °C, decomp.; <sup>1</sup>H NMR (THFd<sup>8</sup>, 25°C, 400 MHz): 7.53-7.47 (m, 3 H, CH<sub>ar</sub>), 7.35-7.26 (m, 3 H, CH<sub>ar</sub>), 7.24-7.00 (m, 8 H, CH<sub>ar</sub>), 6.98-6.83 (m, 2 H, CH<sub>ar</sub>), 2.96 (sept, *J* = 6.8 Hz, 2 H, CHCH<sub>3</sub>), 2.74 (sept, *J* = 6.8 Hz, 2 H, CHCH<sub>3</sub>), 1.26 (d, *J* = 6.8 Hz, 6 H, CH<sub>3</sub>), 1.00 (d, *J* = 6.8 Hz, 6 H, CH<sub>3</sub>), 0.87 (d, *J* = 6.8 Hz, 6 H, CH<sub>3</sub>), 0.83 (d, *J* = 6.8 Hz, 6 H, CH<sub>3</sub>); <sup>13</sup>C NMR (THFd<sup>8</sup>, 25°C, 75 MHz): 201.9 (C<sub>carbene</sub>), 146.1 (C), 145.8 (C), 145.5 (C), 141.4 (C), 141.3 (C), 140.3 (C), 136.6 (C), 134.4 (C), 131.3 (CH<sub>ar</sub>), 130.2 (CH<sub>ar</sub>), 129.8 (CH<sub>ar</sub>), 129.4 (CH<sub>ar</sub>), 128.8 (CH<sub>ar</sub>), 128.5 (CH<sub>ar</sub>), 128.2 (CH<sub>ar</sub>), 126.3 (CH<sub>ar</sub>), 126.1 (CH<sub>ar</sub>), 124.4 (CH<sub>ar</sub>), 29.7 (CHCH<sub>3</sub>), 29.4 (CHCH<sub>3</sub>), 25.7 (CH<sub>3</sub>), 24.3 (CH<sub>3</sub>), 23.9 (CH<sub>3</sub>), 22.8 (CH<sub>3</sub>).

**Synthesis of *a*NHC gold(I) complex 10**

THF (10 mL) was slowly added at -78°C to a solid mixture of *a*NHC **9** (480 mg, 0.88 mmol) and chloro(dimethylsulfide)gold (I) 261 mg (0.88mmol). The reaction mixture was stirred at room temperature for 12 hours. The solvent was removed under vacuum, and CH<sub>2</sub>Cl<sub>2</sub> was added to the solid mixture. After filtration and evaporation

of the solvent under vacuum, the gold complex **10** was obtained as a white solid (535 mg, 79 % yield). Single crystals suitable for an X-ray diffraction study were grown by slow evaporation of a  $\text{CDCl}_3$  solution.

M. p. 267-269°C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 25 °C, 300 MHz): 7.56-7.54 (m, 2 H,  $\text{CH}_{\text{ar}}$ ), 7.47-7.41 (m, 2H,  $\text{CH}_{\text{ar}}$ ), 7.21-7.15 (m, 8 H,  $\text{CH}_{\text{ar}}$ ), 7.07-7.02 (m, 2 H,  $\text{CH}_{\text{ar}}$ ), 6.86 (d,  $J$  = 7.8 Hz, 2H,  $\text{CH}_{\text{ar}}$ ), 2.67-2.54 (m, 4H,  $\text{CHCH}_3$ ), 1.47 (d,  $J$  = 6.6 Hz, 6 H,  $\text{CH}_3$ ), 0.93 (d,  $J$  = 6.6 Hz, 6H,  $\text{CH}_3$ ), 0.79 (d,  $J$  = 6.0 Hz, 12H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 25 °C, 100 MHz): 153.7 (Au-C), 145.1 (C), 144.9 (C), 144.2 (C), 139.6 (C), 135.3 (C), 131.6 ( $\text{CH}_{\text{ar}}$ ), 130.9 ( $\text{CH}_{\text{ar}}$ ), 129.7 ( $\text{CH}_{\text{ar}}$ ), 128.4 ( $\text{CH}_{\text{ar}}$ ), 128.3 ( $\text{CH}_{\text{ar}}$ ), 125.5 ( $\text{CH}_{\text{ar}}$ ), 124.8 ( $\text{CH}_{\text{ar}}$ ), 123.4 (C), 29.1 ( $\text{CHCH}_3$ ), 28.8 ( $\text{CHCH}_3$ ), 25.8 ( $\text{CH}_3$ ), 23.9 ( $\text{CH}_3$ ), 23.6 ( $\text{CH}_3$ ), 22.8 ( $\text{CH}_3$ ).

### Synthesis of *a*NHC-CO<sub>2</sub> adduct **11**

CO<sub>2</sub> was bubbled through a stirred THF solution (10 mL) of *a*NHC **9** (462 mg, 0.86 mmol) at -78°C. Removal of the solvent under vacuum, afforded a white solid. Colorless crystals of **11** (475 mg, 95 % yield) were obtained from a  $\text{CH}_2\text{Cl}_2$ /hexane solution.

M. p. 286-287°C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 25 °C, 300 MHz): 7.48-7.33 (m, 4 H,  $\text{CH}_{\text{ar}}$ ), 7.24-7.15 (m, 8H,  $\text{CH}_{\text{ar}}$ ), 7.05-7.00 (m, 2 H,  $\text{CH}_{\text{ar}}$ ), 6.79 (d,  $J$  = 9 Hz, 2 H,  $\text{CH}_{\text{ar}}$ ), 2.78 (t,  $J$  = 6.5 Hz, 2H,  $\text{CHCH}_3$ ), 2.47 (t,  $J$  = 6.5 Hz, 2 H,  $\text{CHCH}_3$ ), 1.38 (d,  $J$  = 6.5 Hz, 6 H,  $\text{CH}_3$ ), 0.81 (d,  $J$  = 6.5 Hz, 6H,  $\text{CH}_3$ ), 0.74 (d,  $J$  = 6.5 Hz, 6H,  $\text{CH}_3$ ), 0.68 (d,  $J$  = 6.5 Hz, 6H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 25 °C, 100 MHz): 158.9 (CO), 145.2 (C), 141.4 (C), 136.9 (C), 132.0 ( $\text{CH}_{\text{ar}}$ ), 131.6 ( $\text{CH}_{\text{ar}}$ ), 131.2 ( $\text{CH}_{\text{ar}}$ ), 131.1 (C), 130.2 ( $\text{CH}_{\text{ar}}$ ), 129.6 (C), 129.3 ( $\text{CH}_{\text{ar}}$ ), 128.6 ( $\text{CH}_{\text{ar}}$ ), 128.3 ( $\text{CH}_{\text{ar}}$ ), 125.7 ( $\text{CH}_{\text{ar}}$ ), 125.6 (C), 125.1 ( $\text{CH}_{\text{ar}}$ ), 122.1 (C), 29.2 ( $\text{CHCH}_3$ ), 28.9 ( $\text{CHCH}_3$ ), 25.1 ( $\text{CH}_3$ ), 23.9 ( $\text{CH}_3$ ), 23.5 ( $\text{CH}_3$ ), 23.2 ( $\text{CH}_3$ ); HRMS: m/z calculated for  $\text{C}_{40}\text{H}_{45}\text{N}_2\text{O}_2$  585.3476 , found M 585.3478.

### Crystal Structure Determination of compounds **6Br<sup>-</sup>, 8 and 9.**

The Bruker X8-APEX (S2) X-ray diffraction instrument with Mo-radiation was used for data collection. All data frames were collected at low temperatures (T = 100 K) using an  $\omega$ ,  $\phi$ -scan mode (0.3°  $\omega$ -scan width, hemisphere of reflections) and integrated using a Bruker SAINTPLUS software package (S3). The intensity data were corrected for Lorentzian polarization. Absorption corrections were performed using the SADABS program (S4). The SIR97 (S5) software was used for direct methods solution and phase determination, and Bruker SHELXTL \ (S6) for structure refinement and difference Fourier maps. Atomic coordinates, isotropic and anisotropic displacement parameters of all the non-hydrogen atoms of three compounds were refined by means of a full matrix least-squares procedure on F<sup>2</sup>.

**Crystal and structure parameters of 6Br<sup>-</sup>:** size 0.28 x 0.10 x 0.09 mm<sup>3</sup>, monoclinic, space group P 2(1)/n, **a** = 11.983(2) Å, **b** = 25.022(4) Å, **c** = 11.084(2) Å,  $\alpha$  =  $\gamma$  = 90.0°,  $\beta$  = 98.995(2)°, V = 3578.7(11) Å<sup>3</sup>,  $\rho_{\text{calcd}}$  = 1.154 g/cm<sup>3</sup>, Mo-radiation ( $\lambda$  = 0.71073 Å), T = 100(2) K, reflections collected = 19901, independent reflections = 5163 ( $R_{\text{int}}$  = 0.0587), absorption coefficient  $\mu$  = 1.175 mm<sup>-1</sup>; max/min transmission = 0.9016 and 0.7343, 391 parameters were refined and converged at R1 = 0.0463, wR2 = 0.1080, with intensity I>2σ(I), the final difference map was 1.124 and -0.454 e.Å<sup>-3</sup>.

**Crystal and structure parameters of 8:** size 0.58 x 0.54 x 0.50 mm<sup>3</sup>, monoclinic, space group P2(1)/c, **a** = 9.3873(2) Å, **b** = 19.0624(4) Å, **c** = 17.7135(4) Å,  $\alpha$  = 90°,  $\beta$  = 101.0750(10)°,  $\gamma$  = 90°, V = 3110.70(12) Å<sup>3</sup>,  $\rho_{\text{calcd}}$  = 1.155 g/cm<sup>3</sup>, Mo-radiation ( $\lambda$  = 0.71073 Å), T = 100(2) K, reflections collected = 39957, independent reflections = 10399 ( $R_{\text{int}}$  = 0.0162), absorption coefficient  $\mu$  = 0.066 mm<sup>-1</sup>; max/min transmission = 0.9676 and 0.9626, 503 parameters were refined and converged at R1 = 0.0427, wR2 = 0.1150, with intensity I>2σ(I), the final difference map was 0.549 and -0.206 e.Å<sup>-3</sup>.

**Crystal and structure parameters of 9:** size 0.38 x 0.27 x 0.18 mm<sup>3</sup>, triclinic, space group P-1, **a** = 12.768(3) Å, **b** = 16.710(4) Å, **c** = 17.768(7) Å,  $\alpha$  = 106.074(4)°,  $\beta$  = 102.608(4)°,  $\gamma$  = 105.717(3)°, V = 3325.6(16) Å<sup>3</sup>,  $\rho_{\text{calcd}}$  = 1.123 g/cm<sup>3</sup>, Mo-radiation ( $\lambda$  = 0.71073 Å), T = 100(2) K, reflections collected = 35287, independent reflections = 11836 ( $R_{\text{int}}$  = 0.0515), absorption coefficient  $\mu$  = 0.064 mm<sup>-1</sup>; max/min transmission = 0.9885 and 0.9760, 784 parameters were refined and converged at R1 = 0.0476, wR2 = 0.1043, with intensity I>2σ(I), the final difference map was 0.401 and -0.256 e.Å<sup>-3</sup>.

**Crystal and structure parameters of 10:** size 0.25 x 0.16 x 0.10 mm<sup>3</sup>, triclinic, space group P-1, **a** = 9.921(4) Å, **b** = 11.071(5) Å, **c** = 21.625(10) Å,  $\alpha$  = 75.288(7)°,  $\beta$  = 84.508(6)°,  $\gamma$  = 65.951(5)°, V = 2097.8(16) Å<sup>3</sup>,  $\rho_{\text{calcd}}$  = 1.602 g/cm<sup>3</sup>, Mo-radiation ( $\lambda$  = 0.71073 Å), T = 100(2) K, reflections collected = 13615, independent reflections = 8091 ( $R_{\text{int}}$  = 0.0268), absorption coefficient  $\mu$  = 3.984 mm<sup>-1</sup>; max/min transmission = 0.6914 and 0.4358, 497 parameters were refined and converged at R1 = 0.0384, wR2 = 0.1010, with intensity I>2σ(I), the final difference map was 3.451 and -1.787 e.Å<sup>-3</sup>.

### Computational details

The geometries of the molecules have been optimized using gradient-corrected density functional theory at the BP86/def-SVP level (*S7-S9*). The nature of the stationary points was verified by calculation of the vibrational frequencies. Improved single-point energies were calculated with larger basis sets at BP86/def2-TZVPP (*S10*) using BP86/def-SVP optimized geometries. Relative energies in this work are given at BP86/def2-TZVPP//BP86/def-SVP, which include zero-point energy contributions at BP86/def-SVP. Temperature has been considered in the calculated proton affinities. The  $^{13}\text{C}$  NMR chemical shift calculations of **9** were carried out at BP86/def-SVP using the GIAO (*S11*) method. All calculations were done with the program package Gaussian 03 (*S12*).

**Total energies (in a.u.) and Cartesian coordinates (in Å, BP86/def-SVP) using G03 programme package**

**9**

$E_{BP86/\text{def-SVP}} = -1620.92468$

$E + ZPVE_{BP86/\text{def-SVP}} = -1620.21641$

$E_{BP86/\text{def2-TZVPP}/BP86/\text{def-SVP}} = -1622.65337$

C	0.406348000	-1.933398000	-0.027495000
C	0.481239000	0.393983000	-0.000456000
C	-0.893931000	-1.403762000	-0.099729000
N	1.199539000	-0.784173000	0.012773000
N	-0.834802000	0.016682000	-0.059797000
C	1.011745000	1.766797000	0.024240000
C	2.186862000	2.093490000	-0.704601000
C	0.386068000	2.799391000	0.772303000
C	2.710645000	3.394036000	-0.681592000
H	2.689428000	1.322221000	-1.303095000
C	0.913364000	4.099158000	0.787439000
H	-0.518823000	2.581587000	1.354233000
C	2.078506000	4.405790000	0.062775000
H	3.620997000	3.618424000	-1.259616000
H	0.408396000	4.878778000	1.379560000
H	2.491665000	5.426628000	0.078315000
C	-2.122949000	-2.211743000	-0.226005000
C	-2.032256000	-3.577703000	0.159521000
C	-3.362775000	-1.756171000	-0.744833000
C	-3.129233000	-4.439823000	0.042149000
H	-1.065322000	-3.935251000	0.544593000
C	-4.461539000	-2.626409000	-0.858585000
H	-3.481105000	-0.716064000	-1.075320000
C	-4.356434000	-3.970266000	-0.464723000
H	-3.026973000	-5.492259000	0.352983000
H	-5.410228000	-2.243354000	-1.268178000
H	-5.220625000	-4.647559000	-0.554946000
C	-1.950163000	0.937792000	-0.062356000
C	-2.252028000	1.655380000	-1.253648000
C	-2.727856000	1.069503000	1.123211000
C	-3.360353000	2.527070000	-1.226170000
C	-3.826396000	1.952944000	1.085721000
C	-4.141957000	2.677285000	-0.072285000
H	-3.618974000	3.095929000	-2.133519000
H	-4.449028000	2.074064000	1.986430000
H	-5.005353000	3.361498000	-0.076653000
C	2.641057000	-0.880788000	0.134675000
C	3.400440000	-1.195660000	-1.024473000
C	3.236217000	-0.714499000	1.412950000
C	4.797758000	-1.313620000	-0.875649000

C	4.638523000	-0.837704000	1.500817000
C	5.413824000	-1.129531000	0.370165000
H	5.415632000	-1.555040000	-1.754266000
H	5.131599000	-0.711713000	2.476725000
H	6.507972000	-1.221218000	0.462072000
C	-2.421144000	0.303842000	2.414460000
C	-3.596836000	-0.607701000	2.829011000
C	-2.036628000	1.255855000	3.568860000
H	-1.549117000	-0.353633000	2.218844000
H	-3.874002000	-1.307370000	2.015960000
H	-3.320836000	-1.209628000	3.720019000
H	-4.497594000	-0.013935000	3.095146000
H	-1.146600000	1.871509000	3.324702000
H	-2.866914000	1.949300000	3.820998000
H	-1.799593000	0.674617000	4.484508000
C	-1.451004000	1.494429000	-2.548109000
C	-0.865480000	2.837602000	-3.032786000
C	-2.295902000	0.822677000	-3.653310000
H	-0.596751000	0.818831000	-2.336007000
H	-0.238220000	3.314547000	-2.252870000
H	-0.233594000	2.680059000	-3.931925000
H	-1.665503000	3.555428000	-3.314072000
H	-2.675980000	-0.168638000	-3.333201000
H	-3.170261000	1.447824000	-3.934391000
H	-1.685391000	0.672072000	-4.568434000
C	2.391027000	-0.512760000	2.671540000
C	3.048476000	0.401442000	3.721152000
C	2.018316000	-1.890106000	3.268426000
H	1.443566000	-0.021882000	2.364090000
H	3.347602000	1.377530000	3.286735000
H	2.339262000	0.599417000	4.551712000
H	3.950490000	-0.061806000	4.174671000
H	1.497153000	-2.517398000	2.515791000
H	2.929581000	-2.433414000	3.598202000
H	1.353121000	-1.770336000	4.150110000
C	2.738167000	-1.452256000	-2.379410000
C	2.471712000	-2.964330000	-2.559636000
C	3.528986000	-0.872258000	-3.567821000
H	1.746180000	-0.950995000	-2.363289000
H	1.822423000	-3.332243000	-1.738175000
H	1.964032000	-3.159241000	-3.528432000
H	3.424993000	-3.535277000	-2.549429000
H	3.748555000	0.208660000	-3.438211000
H	4.496523000	-1.395519000	-3.721501000
H	2.947976000	-0.990599000	-4.506156000

**6 (9.H+)**

$E_{BP86/\text{def-SVP}} = -1621.39753$

$E + ZPVE_{BP86/\text{def-SVP}} = -1620.67568$

$E_{BP86/\text{def2-TZVPP}/BP86/\text{def-SVP}} = -1623.12424$

C	0.352748000	-1.868278000	-0.129413000
C	0.475815000	0.365936000	0.027812000
C	-0.946957000	-1.398808000	-0.165484000
N	1.209443000	-0.786819000	-0.015448000
N	-0.845809000	0.002826000	-0.065569000
C	1.016497000	1.729166000	0.152478000
C	2.197030000	2.093766000	-0.544218000
C	0.378763000	2.695849000	0.970235000
C	2.719861000	3.389125000	-0.424358000
H	2.700466000	1.368223000	-1.196347000
C	0.910530000	3.988248000	1.086365000
H	-0.529375000	2.434113000	1.528430000
C	2.080690000	4.340195000	0.390670000
H	3.632787000	3.658039000	-0.977507000
H	0.406982000	4.724746000	1.731117000
H	2.494697000	5.356256000	0.483401000
C	-2.181283000	-2.199639000	-0.261967000
C	-2.203712000	-3.466453000	0.375907000
C	-3.318427000	-1.788211000	-0.998609000
C	-3.327864000	-4.298341000	0.274999000
H	-1.340420000	-3.791432000	0.977424000
C	-4.442206000	-2.624404000	-1.091870000
H	-3.325577000	-0.817527000	-1.512104000
C	-4.452448000	-3.879163000	-0.458257000
H	-3.329623000	-5.275840000	0.781572000
H	-5.316611000	-2.292147000	-1.672489000
H	-5.337055000	-4.530230000	-0.534687000
C	-1.971552000	0.927100000	-0.094350000
C	-2.202208000	1.677993000	-1.280777000
C	-2.802663000	1.018851000	1.057069000
C	-3.310678000	2.550385000	-1.279771000
C	-3.895024000	1.908242000	0.987939000
C	-4.148593000	2.666697000	-0.162754000
H	-3.522535000	3.149230000	-2.179189000
H	-4.562006000	2.006416000	1.858361000
H	-5.008670000	3.353718000	-0.190209000
C	2.653025000	-0.937543000	0.109635000
C	3.401548000	-1.229143000	-1.064168000
C	3.233399000	-0.842536000	1.401931000
C	4.790222000	-1.412380000	-0.905985000
C	4.629586000	-1.025923000	1.488212000
C	5.399930000	-1.306923000	0.352321000
H	5.408157000	-1.640774000	-1.788007000

H	5.120719000	-0.955486000	2.471169000
H	6.487357000	-1.450774000	0.448492000
C	-2.574190000	0.217314000	2.343338000
C	-3.772278000	-0.707529000	2.654440000
C	-2.274395000	1.136699000	3.548892000
H	-1.684127000	-0.430670000	2.194672000
H	-4.002216000	-1.383665000	1.807586000
H	-3.553898000	-1.332122000	3.545066000
H	-4.687106000	-0.120245000	2.879348000
H	-1.381830000	1.774177000	3.382538000
H	-3.129272000	1.808082000	3.772531000
H	-2.085827000	0.528692000	4.457654000
C	-1.335780000	1.575492000	-2.539727000
C	-0.713772000	2.938832000	-2.912930000
C	-2.126612000	0.987324000	-3.730105000
H	-0.497956000	0.876279000	-2.330891000
H	-0.134230000	3.370487000	-2.072666000
H	-0.031803000	2.826360000	-3.780897000
H	-1.492789000	3.675380000	-3.200610000
H	-2.531904000	-0.020426000	-3.505575000
H	-2.979131000	1.638750000	-4.014677000
H	-1.470033000	0.893988000	-4.619813000
C	2.423478000	-0.594779000	2.675579000
C	2.893081000	0.673726000	3.419337000
C	2.453030000	-1.834349000	3.597827000
H	1.363549000	-0.429881000	2.386686000
H	2.850013000	1.569095000	2.766665000
H	2.250931000	0.861734000	4.304432000
H	3.935623000	0.570830000	3.785955000
H	2.071514000	-2.739738000	3.082500000
H	3.483283000	-2.056930000	3.945492000
H	1.827480000	-1.662897000	4.498206000
C	2.765257000	-1.370935000	-2.450143000
C	2.725303000	-2.852104000	-2.891491000
C	3.468249000	-0.504242000	-3.516588000
H	1.714233000	-1.014921000	-2.382439000
H	2.190238000	-3.492290000	-2.160662000
H	2.214539000	-2.954265000	-3.871178000
H	3.750593000	-3.263051000	-3.001491000
H	3.496893000	0.567963000	-3.232481000
H	4.513375000	-0.832085000	-3.693064000
H	2.934397000	-0.582472000	-4.485879000
H	0.736320000	-2.890292000	-0.191438000

**9-H<sub>2</sub><sup>2+</sup>**E<sub>BP86/def-SVP</sub> = -1621.63600E +ZPVE<sub>BP86/def-SVP</sub> = -1620.90422E<sub>BP86/def2-TZVPP//BP86/def-SVP</sub> = -1623.36453

C	-0.427283000	1.896157000	0.350323000
C	-0.474777000	-0.357962000	-0.087588000
C	0.978603000	1.398165000	0.185190000
N	-1.248442000	0.709578000	0.116506000
N	0.892088000	0.056521000	-0.023904000
C	-0.928402000	-1.713103000	-0.364885000
C	-2.107865000	-1.898613000	-1.145559000
C	-0.241257000	-2.857008000	0.135668000
C	-2.567346000	-3.187968000	-1.428150000
H	-2.643952000	-1.033875000	-1.557347000
C	-0.732416000	-4.140286000	-0.129950000
H	0.652183000	-2.744756000	0.761284000
C	-1.887704000	-4.311730000	-0.916194000
H	-3.463878000	-3.321031000	-2.052387000
H	-0.208749000	-5.016539000	0.281120000
H	-2.261540000	-5.325166000	-1.131019000
C	2.131889000	2.256527000	0.199287000
C	1.927745000	3.621782000	0.595800000
C	3.449414000	1.855816000	-0.202635000
C	2.982053000	4.532737000	0.594642000
H	0.936879000	3.970714000	0.922965000
C	4.490734000	2.785593000	-0.220789000
H	3.647277000	0.824135000	-0.515456000
C	4.267443000	4.119077000	0.181251000
H	2.811121000	5.571972000	0.913611000
H	5.493724000	2.470825000	-0.546438000
H	5.099481000	4.841120000	0.174836000
C	2.019855000	-0.859877000	-0.170032000
C	2.344470000	-1.317373000	-1.477797000
C	2.730957000	-1.234995000	1.007865000
C	3.447287000	-2.191000000	-1.580923000
C	3.818418000	-2.113169000	0.823844000
C	4.175792000	-2.583584000	-0.449071000
H	3.742329000	-2.570245000	-2.571285000
H	4.397281000	-2.439574000	1.701737000
H	5.032924000	-3.265877000	-0.558981000
C	-2.694552000	0.788689000	0.286818000
C	-3.449546000	1.404998000	-0.751739000
C	-3.260139000	0.326952000	1.508128000
C	-4.835343000	1.535495000	-0.535686000
C	-4.655016000	0.483714000	1.650002000
C	-5.433266000	1.078339000	0.647905000
H	-5.461153000	2.000584000	-1.312463000

H	-5.140653000	0.139797000	2.576354000
H	-6.518983000	1.190030000	0.791787000
C	2.381724000	-0.757821000	2.422281000
C	3.529493000	0.071377000	3.042677000
C	2.005755000	-1.937090000	3.349329000
H	1.488804000	-0.095809000	2.362080000
H	3.814573000	0.936310000	2.410007000
H	3.229034000	0.459712000	4.037086000
H	4.437884000	-0.547763000	3.192261000
H	1.147634000	-2.523856000	2.962164000
H	2.857409000	-2.634516000	3.485660000
H	1.728047000	-1.559270000	4.354256000
C	1.602490000	-0.879520000	-2.743206000
C	1.069755000	-2.086720000	-3.543892000
C	2.491794000	0.026648000	-3.626781000
H	0.720129000	-0.272094000	-2.440231000
H	0.426727000	-2.742524000	-2.922926000
H	0.474250000	-1.737519000	-4.411610000
H	1.896707000	-2.707066000	-3.945752000
H	2.837857000	0.930028000	-3.083749000
H	3.390307000	-0.517709000	-3.983491000
H	1.930494000	0.362762000	-4.522305000
C	-2.453308000	-0.283106000	2.655985000
C	-2.890177000	-1.735571000	2.947702000
C	-2.535693000	0.594494000	3.926218000
H	-1.381038000	-0.319081000	2.357088000
H	-2.814563000	-2.378548000	2.047176000
H	-2.257526000	-2.177826000	3.744141000
H	-3.940395000	-1.776983000	3.302462000
H	-2.206307000	1.637542000	3.736478000
H	-3.571758000	0.643519000	4.318990000
H	-1.898773000	0.173171000	4.730640000
C	-2.825904000	1.915510000	-2.055286000
C	-2.793336000	3.461490000	-2.093061000
C	-3.535881000	1.357474000	-3.308326000
H	-1.773465000	1.550139000	-2.098515000
H	-2.267290000	3.901992000	-1.217976000
H	-2.292100000	3.821910000	-3.014509000
H	-3.820273000	3.881425000	-2.085322000
H	-3.574707000	0.248739000	-3.310101000
H	-4.577853000	1.728147000	-3.388667000
H	-3.004227000	1.679778000	-4.226519000
H	-0.632498000	2.285900000	1.373893000
H	-0.685645000	2.707439000	-0.365418000

**Normal NHC isomer of 9** $E_{BP86/def-SVP} = -1620.94629$  $E +ZPVE_{BP86/def-SVP} = -1620.23824$  $E_{BP86/def2-TZVPP//BP86/def-SVP} = -1622.67561$ 

N	1.070924000	-0.541555000	0.086870000
N	-1.070643000	-0.543103000	-0.076452000
C	0.692819000	0.822326000	0.045661000
C	-0.693194000	0.821385000	-0.053529000
C	0.000348000	-1.404047000	0.010605000
C	-1.631874000	1.961941000	-0.057599000
C	-1.452701000	3.024968000	0.863927000
H	-0.620768000	2.978730000	1.583133000
C	-2.326988000	4.122021000	0.875740000
H	-2.169579000	4.935411000	1.601977000
C	-3.405253000	4.179441000	-0.025955000
H	-4.094851000	5.038373000	-0.013032000
C	-3.597972000	3.130105000	-0.941371000
H	-4.438424000	3.164822000	-1.652720000
C	-2.721125000	2.033451000	-0.960813000
H	-2.878946000	1.224314000	-1.688324000
C	-2.432971000	-1.029215000	-0.107371000
C	-3.215093000	-0.970153000	1.076366000
C	-4.539237000	-1.453052000	1.015327000
H	-5.166081000	-1.421389000	1.920472000
C	-5.065019000	-1.983255000	-0.169846000
H	-6.101225000	-2.356959000	-0.195308000
C	-4.268467000	-2.045755000	-1.321760000
H	-4.686619000	-2.474592000	-2.245696000
C	-2.941141000	-1.569703000	-1.320824000
C	2.433672000	-1.026623000	0.120268000
C	2.947521000	-1.546340000	1.340436000
C	4.274560000	-2.022988000	1.343087000
H	4.697327000	-2.435805000	2.272139000
C	5.065463000	-1.980909000	0.186287000
H	6.101485000	-2.355028000	0.213117000
C	4.534607000	-1.469864000	-1.004950000
H	5.157399000	-1.453084000	-1.913315000
C	3.210455000	-0.987071000	-1.067701000
C	-2.650182000	-0.478228000	2.409409000
H	-1.670284000	0.000195000	2.205792000
C	-3.544909000	0.581377000	3.082949000
H	-3.726203000	1.445872000	2.412509000
H	-3.062435000	0.961369000	4.008062000
H	-4.531352000	0.164153000	3.377819000
C	-2.385830000	-1.676188000	3.348859000
H	-3.330067000	-2.205646000	3.598700000
H	-1.927596000	-1.334795000	4.301532000

H	-1.700942000	-2.409756000	2.877568000
C	-2.080488000	-1.693276000	-2.578962000
H	-1.229283000	-0.988807000	-2.467051000
C	-2.830270000	-1.311115000	-3.870483000
H	-3.639767000	-2.031607000	-4.113423000
H	-2.130565000	-1.310777000	-4.732304000
H	-3.287830000	-0.301659000	-3.804452000
C	-1.483104000	-3.115396000	-2.675188000
H	-2.288107000	-3.878474000	-2.742719000
H	-0.864922000	-3.332996000	-1.780570000
H	-0.844404000	-3.212620000	-3.578863000
C	2.092258000	-1.647122000	2.604322000
H	1.248130000	-0.934522000	2.488989000
C	1.480421000	-3.061764000	2.719160000
H	0.856676000	-3.283078000	1.829243000
H	0.844418000	-3.142033000	3.626403000
H	2.277946000	-3.832140000	2.792255000
C	2.852244000	-1.258972000	3.887986000
H	3.653772000	-1.986581000	4.136031000
H	2.156397000	-1.239899000	4.752679000
H	3.321976000	-0.256122000	3.808102000
C	2.640515000	-0.514585000	-2.405629000
H	1.659170000	-0.037560000	-2.205785000
C	2.378547000	-1.725041000	-3.329441000
H	3.323878000	-2.254816000	-3.574356000
H	1.917628000	-1.397140000	-4.285548000
H	1.696690000	-2.454525000	-2.847506000
C	3.529860000	0.540107000	-3.094043000
H	3.707455000	1.414452000	-2.435478000
H	3.045116000	0.905207000	-4.023958000
H	4.518115000	0.123464000	-3.383622000
C	1.631216000	1.963055000	0.035192000
C	1.453009000	3.013892000	-0.900424000
C	2.719638000	2.046346000	0.938389000
C	2.327574000	4.110527000	-0.925865000
H	0.621704000	2.958405000	-1.619710000
C	3.596708000	3.142501000	0.905372000
H	2.876611000	1.246966000	1.676787000
C	3.405078000	4.179590000	-0.024081000
H	2.170975000	4.914348000	-1.662854000
H	4.436455000	3.186505000	1.617037000
H	4.094799000	5.038196000	-0.047724000

**8** $E_{BP86/def-SVP} = -1620.93913$  $E + ZPVE_{BP86/def-SVP} = -1620.23016$  $E_{BP86/def2-TZVPP//BP86/def-SVP} = -1622.66373$ 

N	0.790812000	0.079185000	-0.371238000
N	-1.498851000	0.502173000	0.027450000
C	-0.776372000	1.707123000	0.038127000
C	0.555664000	1.484829000	-0.155591000
C	-0.569874000	-0.586775000	-0.447569000
C	-1.144781000	-0.874489000	-1.946906000
C	-2.618570000	-0.523065000	-1.728903000
C	-3.739951000	-0.866809000	-2.489499000
C	-4.991645000	-0.318174000	-2.138331000
C	-5.104088000	0.557429000	-1.046454000
C	-3.989763000	0.913047000	-0.247656000
C	-2.752073000	0.351623000	-0.629013000
C	1.576777000	2.536328000	-0.233905000
C	1.390024000	3.768842000	0.450965000
C	2.314452000	4.814428000	0.324679000
C	3.465533000	4.658325000	-0.471092000
C	3.669589000	3.441913000	-1.145441000
C	2.739163000	2.398016000	-1.029997000
C	-0.729431000	-1.839433000	0.436136000
C	0.145185000	-2.944084000	0.331358000
C	-0.050271000	-4.105120000	1.097685000
C	-1.141849000	-4.199910000	1.977396000
C	-2.024284000	-3.113460000	2.089526000
C	-1.813615000	-1.945682000	1.335715000
C	-0.578501000	0.146045000	-2.966872000
C	-0.961372000	-2.296593000	-2.494989000
C	1.946894000	-0.522511000	0.284820000
C	2.088213000	-0.476603000	1.710249000
C	3.258018000	-1.001910000	2.298411000
C	4.268958000	-1.589491000	1.531554000
C	4.118121000	-1.654339000	0.142776000
C	2.981967000	-1.125583000	-0.505190000
C	1.032750000	0.103457000	2.657193000
C	0.608195000	-0.913126000	3.739743000
C	1.523606000	1.411509000	3.316666000
C	2.936490000	-1.251164000	-2.032336000
C	4.153909000	-0.596296000	-2.725403000
C	2.848901000	-2.724864000	-2.492341000
C	-4.125220000	1.840459000	0.958196000
C	-5.242730000	1.392320000	1.922771000
C	-4.327257000	3.309116000	0.523400000
H	-1.294997000	2.667594000	0.122432000
H	-3.652441000	-1.545231000	-3.353345000

H	-5.888870000	-0.580765000	-2.720882000
H	-6.095260000	0.966306000	-0.791442000
H	0.513497000	3.895906000	1.105436000
H	2.142964000	5.758056000	0.867488000
H	4.198123000	5.476067000	-0.558413000
H	4.562702000	3.304237000	-1.776505000
H	2.894702000	1.462434000	-1.579492000
H	0.999562000	-2.904821000	-0.354297000
H	0.658240000	-4.942929000	0.999793000
H	-1.300718000	-5.113054000	2.572890000
H	-2.883675000	-3.166355000	2.776875000
H	-2.500004000	-1.096808000	1.454333000
H	-1.131581000	0.051892000	-3.924178000
H	0.494793000	-0.036541000	-3.171199000
H	-0.686467000	1.190474000	-2.615603000
H	-1.444477000	-3.062386000	-1.858425000
H	0.108832000	-2.556709000	-2.607193000
H	-1.412808000	-2.363093000	-3.507828000
H	3.370362000	-0.958572000	3.393376000
H	5.170722000	-1.998141000	2.015085000
H	4.910923000	-2.119948000	-0.464726000
H	0.130007000	0.342614000	2.063512000
H	0.279906000	-1.873856000	3.297080000
H	-0.236297000	-0.505256000	4.334667000
H	1.433723000	-1.128404000	4.451332000
H	2.403438000	1.224731000	3.969256000
H	0.725114000	1.849889000	3.952665000
H	1.820080000	2.167913000	2.563979000
H	2.020524000	-0.724306000	-2.368205000
H	4.315364000	0.451895000	-2.406332000
H	4.019983000	-0.600947000	-3.827809000
H	5.090464000	-1.151683000	-2.506590000
H	3.769679000	-3.283042000	-2.219331000
H	2.738582000	-2.785128000	-3.595838000
H	1.993720000	-3.266631000	-2.041090000
H	-3.166488000	1.779897000	1.518877000
H	-6.246134000	1.461931000	1.451872000
H	-5.258959000	2.036336000	2.827195000
H	-5.098960000	0.342904000	2.252511000
H	-3.511486000	3.658151000	-0.143334000
H	-4.364944000	3.984724000	1.404301000
H	-5.279731000	3.429189000	-0.035629000

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